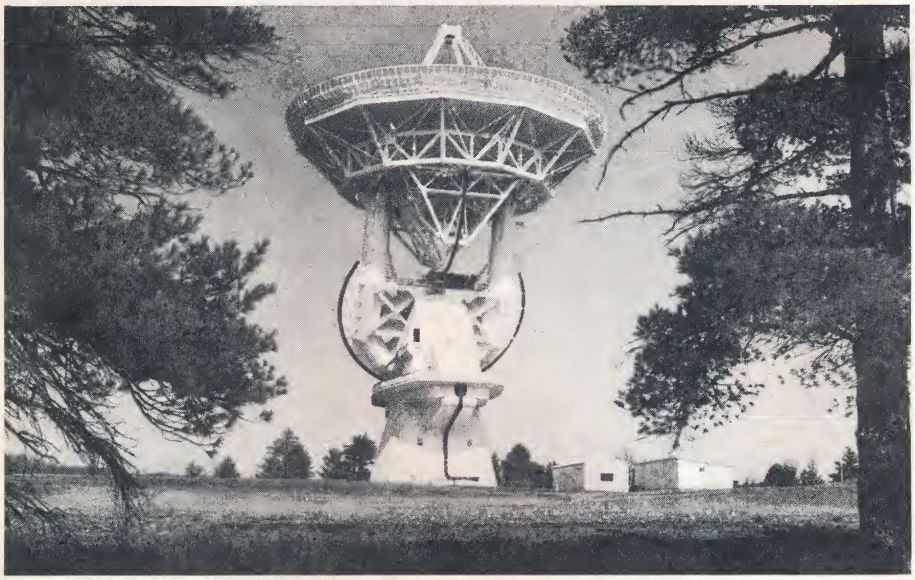
NSRDS **Reference data report**

an informal communication of the National Standard Reference Data System

Office of Standard Reference Data | U.S. DEPARTMENT OF COMMERCE | National Bureau of Standards | MAY/JUN 1979

NBS Molecular Spectra Data Center Aids Identification of Interstellar Molecules



Spectra from interstellar matter are observed with telescopes such as the 140 ft. radio telescope at Green Bank, W.VA. Some of the first molecules observed were detected on this system.

Nearly fifty molecular species have been found in the interstellar clouds of gas and "dust" which comprise roughly 20 percent of the mass of our galaxy, the Milky Way. The majority of these interstellar molecules have been identified via their characteristic spectra in the radio and microwave frequency regions. The OH molecule was the first discovered by radio astronomers.[1] This occurred in 1963 and it took five years before a second was observed, the ammonia molecule (NH_3). Rather rapidly after the ammonia discovery, a series of detections of other inorganic, e.g., H_2O, and organic, e.g., H_2CO, CO, CH_3OH, molecules were reported. These interstellar species were usually identified by observing the absorption or emission of radiation in the microwave region at frequencies unique to each molecule.

The rapid growth of molecule radio astronomy occurred because of the availability of a large body of microwave spectral laboratory data. The NBS Monograph 70 series of Microwave Spectral Tables, published in the early 1960's, was heavily used as a guide to searches for the identification of interstellar molecules. Since that monograph appeared, more than four times the number of species listed in the earlier tables have been analyzed. The Molecular Spectra Data Center has

(continued on page 2)

NEWS BRIEFS

Atomic data evaluation activities in Japan related to nuclear fusion research are being coordinated by the Institute of Plasma Physics at Nagoya University. Plans for data compilations include electron excitation and ionization of atomic ions, charge transfer data, recombination coefficients and related data, and update of data on hydrogen and helium ions. The Nagoya Data Center is part of the IAEA Atomic and Molecular Data Center Network. Several compilations are already being prepared. For further information contact:

Research Information Center
IPP/Nagoya University
Nagoya 464, Japan

The Thermodynamics Research Center (TRC) at Texas A & M University has a new director. Dr. Kenneth R. Hall, presently Professor of Chemical Engineering at Texas A & M, also will serve as director of the Center. Dr. Hall replaces Dr. Bruno Zwolinski, who established TRC in 1961 and was its director until 1978.

Atomic spectroscopy tables, representing a completely new set of spectroscopic data, have been published in the Chemical Rubber Company's 59th edition of the Handbook of Chemistry and Physics, after having had no spectroscopic data in several editions. They contain wavelengths for 42,000 lines of 98 elements for up to four times ionized atoms and

(continued on page 3)

NBS Molecular Spectra Data Center *(continued)*

produced two parts of a revised series of Microwave Spectral Tables[2,3] which are used by astronomers and laboratory spectroscopists.

Since the requirements of molecular radio astronomy differ substantially from those of laboratory studies, NBS also has developed a series of spectral tables[4-17] oriented to known interstellar molecules and information required to interpret astronomical observations. Perhaps the most important and unique element of the spectral reviews is the inclusion of calculated, i.e., predicted, spectral lines and the uncertainties in these transitions which have not been measured in the laboratory. These are now widely used by astronomers, both as a guide to further observations of known interstellar molecules and as a means of assigning unidentified interstellar lines often observed accidentally. Approximately 30 percent of such observations have been identified by using these spectral tables. Through new measurements and spectral calculations carried out as part of the review process, the unique combination of microwave spectroscopy laboratory facilities and the data center activities has contributed to identifying such new interstellar molecules as SO_2, H_2CNH, NH_2CN, CH_3OCH_3, CH_3CH_2OH, and CH_3CH_2CN.

In recent years, there has been a growing need to consolidate the several hundred observed interstellar molecule radio lines and to develop a list of accurate frequencies for them. Accurate transition frequencies are needed for deriving the molecular cloud velocity (Doppler shift) for each of the species since this is a physical parameter allowing correlation of observations of various species and interstellar chemistry. The Data Center has just completed a compilation[18] entitled "Recommended Rest Frequencies for Observed Interstellar Molecular Transitions." This table is used as a guide for system tests involving observations of known molecular lines. We anticipate that it will also facilitate sorting out the known from the unknown as astronomers search for new species.

Additional information can be obtained from:

Dr. F.J. Lovas
Molecular Spectra Data Center
Center for Thermodynamics
and Molecular Science
National Bureau of Standards
Washington, D.C. 20234

1. Radio Observations of OH in the Interstellar Medium, S. Weinreb, A. H. Barrett, M. L. Meeks, and J. C. Henry, Nature 200, 829 (1963).
2. Microwave Spectral Tables, I. Diatomic Molecules, F. J. Lovas and E. Tiemann, J. Phys. Chem. Ref. Data 3, 609 (1974).
3. Microwave Spectral Tables, II. Triatomic Molecules, F. J. Lovas, Ibid., 7, 1445 (1978).
4. Microwave Spectra of Molecules of Astrophysical Interest, I. Formaldehyde, Formamide, and Thioformaldehyde, D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff, Ibid., 1, 1011 (1972).
5. Microwave Spectra of Molecules of Astrophysical Interest, II. Methylenimine, W. H. Kirchhoff, D. R. Johnson, and F. J. Lovas, Ibid., 2, 1 (1973).
6. Microwave Spectra of Molecules of Astrophysical Interest, III. Methanol, R. M. Lees, F. J. Lovas, W. H. Kirchhoff, and D. R. Johnson, Ibid., 2, 205 (1973).
7. Microwave Spectra of Molecules of Astrophysical Interest, IV. Hydrogen Sulfide, P. Helminger, F. C. De Lucia, and W. H. Kirchhoff, Ibid., 2, 215 (1973).
8. Microwave Spectra of Molecules of Astrophysical Interest, V. Water Vapor F. C. De Lucia, P. Helminger, and W. H. Kirchhoff, Ibid., 3, 211 (1974).
9. Microwave Spectra of Molecules of Astrophysical Interest, VI. Carbonyl Sulfide and Hydrogen Cyanide, A. G. Maki, Ibid., 3, 221 (1974).
10. Microwave Spectra of Molecules of Astrophysical Interest, VII. Carbon Monoxide, Carbon Monosulfide, and Silicon Monoxide, F. J. Lovas and P. H. Krupenie, Ibid., 3, 245 (1974).
11. Microwave Spectra of Molecules of Astrophysical Interest, VIII. Sulfur Monoxide, E. Tiemann, Ibid., 3, 259 (1974).
12. Microwave Spectra of Molecules of Astrophysical Interest, IX. Acetaldehyde, A. Bauder, F. J. Lovas, and D. R. Johnson, Ibid., 5, 53 (1976).
13. Microwave Spectra of Molecules of Astrophysical Interest, X. Isocyanic Acid, G. Winnewisser, W. H. Hocking, and M. C. L. Gerry, Ibid., 5, 79 (1976).
14. Microwave Spectra of Molecules of Astrophysical Interest, XI. Silicon Sulfide, E. Tiemann, Ibid., 5, 1147 (1976).
15. Microwave Spectra of Molecules of Astrophysical Interest, XII. Hydroxyl Radical, R. A. Beaudet and R. L. Poynter, Ibid., 7, 311 (1978).
16. Microwave Spectra of Molecules of Astrophysical Interest, XIII. Cyanoacetylene, W. J. Lafferty and F. J. Lovas, Ibid., 7, 441 (1978).
17. Microwave Spectra of Molecules of Astrophysical Interest, XIV. Vinyl Cyanide (Acrylonitrile), M. C. L. Gerry, K. Yamada, and G. Winnewisser, Ibid., 8, (1979).
18. Recommended Rest Frequencies for Observed Interstellar Molecular Transitions, F. J. Lovas, L. E. Snyder, and D. R. Johnson, Astrophys. J. Suppl., to be published Nov. 1979.

(References 4-16 are available from ACS, 1155 16th St., N.W., Washington, D.C. 20036, as JPCRD Reprint Package O.) □

NSRDS **National Standard Reference Data System**

Reference Data Report

Vol. 3, No. 3 MAY/JUN 1979

Reference Data Report is an informal communication of the National Standard Reference Data System (NSRDS) for the exchange of news and ideas about data centers, publications, meetings, and other activities related to data evaluation and dissemination. The NSRDS, which operates under the authority given in Public Law 90-396, was established to make critically evaluated data in the physical sciences available to the scientific and technical community. The NSRDS is administered and coordinated by the NBS Office of Standard Reference Data. Comments and suggestions on Reference Data Report should be addressed to:

S. P. Fivozinsky,
Office of Standard
Reference Data,
National Bureau of
Standards,
Washington, D. C. 20234

OSRD Activities

The new NSRDS Publication List, 1964-1979, is available on request from:

Office of Standard Reference Data
Reference Center
Building 221 - Room A320
National Bureau of Standards
Washington, D.C. 20234

The Office of Standard Reference Data organized a meeting on May 21, 1979 to discuss interactions between the Chemical Abstracts Service (CAS) of the American Chemical Society (ACS) and Government agencies concerned with computerized chemical data bases. The meeting was attended by top officials of the American Chemical Society and representatives of the Environmenatal Protection Agency, National Institutes of Health, National Science Foundation, and National Library of Medicine. OSRD is working with these agencies to develop new means of disseminating computer-formatted reference data. A crucial aspect of these interagency plans is the standardization of the method of identifying individual chemical substances. Discussion at the meeting centered on the Chemical Abstracts Service's Chemical Registry System, which provides a unique identifier for every chemical substance in machine-readable form; almost 5 million substances are now included. Several agencies which have responsibility for collecting and disseminating data on chemicals are making use of this system. This meeting provided an opportunity for open discussion of ACS plans for future development of the Registry System and agency needs for CAS services. □

NEWS BRIEFS *(continued)*

about 4500 atomic transition probability data for the more prominent transitions of lighter elements up to nickel. The transitions span the wavelength range from the vacuum ultraviolet to the far infrared. The tables, which cover about 160 pages in the new handbook, are probably the most complete and up-to-date tabulation of wavelengths for atomic spectral lines.

The new compilations were edited and assembled by scientists from the Atomic and Plasma Radiation Division at NBS, who also are associated with the Atomic Energy Levels and Atomic Transition Probabilities Data Centers. The data were obtained in cooperation with many collaborators from laboratories throughout the United States.

The newly established International Journal of Thermophysics will be available in 1980. A medium for the publication of papers on experimental and theoretical studies, the Journal will cover thermal and related properties of matter in the solid, liquid, gaseous, and plasma states. The approach will be interdisciplinary, reflecting interests in the various fields of science and engineering related to thermophysical properties and to thermophysics and its applications. The Journal will attempt to satisfy the needs of both generators and users of thermophysical properties data, thus serving as a focal point for scientific communication in this area.

Topics appropriate for publication will include thermodynamic, transport and thermal radiative properties; review of current thermophysics topics; new developments in experimental techniques, instrumentation, and reference materials; methods of collection, critical evaluation, correlation and dissemination of thermophysical properties data and information; as well as international sources for such collections and selected technological applications of thermophysics.

All publications will be refereed by an international board of editors. Articles will appear in English. Members of the international community of researchers are invited to submit brief manuscript abstracts, intended for publication in the first and subsequent issues of the Journal to:

Dr. Ared Cezairliyan
Editor-in-Chief
Thermophysics Division
(Bldg. 236)
National Bureau of Standards
Washington, D.C. 20234 U.S.A.
Telephone: (301) 921-3687

Available on a quarterly basis for $58. per year, all subscription requests should be directly addressed to: Plenum Publishing Co., 227 West 17th Street, New York, NY 10011. □

New Publications

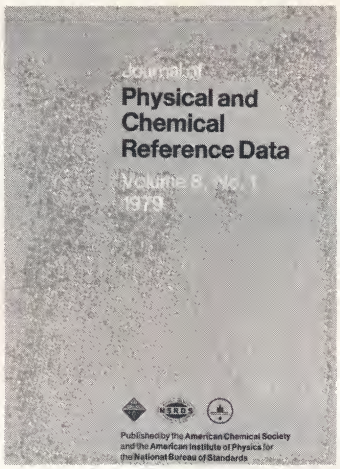
Rate Constants for Reactions of Inorganic Radicals in Aqueous Solution, Alberta B. Ross and Pedatsur Neta, NSRDS-NBS 65, 62 p., 1979. GPO* Stock Number 003-003-02072-9, $3.50.

Bibliography of Low Energy Electron and Photon Cross Section Data (January 1975 through December 1977). J. W. Gallagher, J. R. Rumble, and E. C. Beaty, NBS-SP 426, Suppl. 1, 115 p., 1979. GPO* Stock Number 003-003-02074-5, $4.00.

(continued on page 4)

Articles Appearing in Journal of Physical and Chemical Reference Data

Bound reprints of each paper are available at the indicated price from Business Operations, Books and Journals Division, American Chemical Society, 1155 Sixteenth Street, N.W., Washington, D.C. 20036. Single issue copies of the **Journal** are available for $25.00. Checks payable to the American Chemical Society must accompany the order.



Atomic Radiative and Radiationless Yields for K and L Shells, M. O. Krause, Vol. 8, No. 2, pp. 307-327, $4.00, Reprint #136.

Natural Widths of Atomic K and L Levels, Kα X-Ray Lines and Several KLL Auger Lines, M. O. Krause and J. H. Oliver, Vol. 8, No. 2, pp. 329-338, $3.00, Reprint #137.

Electrical Resistivity of Alkali Elements, T. C. Chi, Vol. 8, No. 2, pp. 339-438, $6.50, Reprint #138.

Electrical Resistivity of Alkaline Earth Elements, T. C. Chi, Vol. 8, No. 2, pp. 439-497, $5.00, Reprint #139.

Vapor Pressures and Boiling Points of Selected Halomethanes, A. P. Kudchadker, S. A. Kudchacker, R. P. Shukla, and P. R. Patnaik, Vol. 8, No. 2, pp. 499-517, $4.00, Reprint #140.

Ideal Gas Thermodynamic Properties of Selected Bromoethanes and Iodoethane, S. A. Kudchadker and A. P. Kudchadker, Vol. 8, No. 2, pp. 519 - 526, $3.00, Reprint #141.

Thermodynamic Properties of Normal and Deuterated Naphthalenes, S. S. Chen, S. A. Kudchadker, and R. C. Wilhoit, Vol.8, No. 2, pp. 527-535, $3.00, Reprint #142.

New Publications *(continued)*

A Bibliography of Sources of Experimental Data Leading to Thermal Properties of Binary Aqueous Electrolyte Solutions, David Smith-Magowan and Robert N. Goldberg, NBS-SP 537, 89 p., 1979. GPO* Stock Number 003-003-02033-8, $2.75.

*Order from Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. (Add 25% for other than U.S. mailing.) □

Microwave Spectra of Molecules of Astrophysical interest. XV. Propyne, A. Bauer, D. Boucher, J. Burie, J. Demaison, and A. Dubrulle, Vol. 8, No. 2, pp. 537-558, $4.00, Reprint #143.

A Correlation of the Viscosity and Thermal Conductivity Data of Gaseous and Liquid Propane, P. M. Holland, H. J. M. Hanley, K. E. Gubbins, and J. M. Haile, Vol. 8, No. 2, pp. 559-575, $4.00, Reprint #144. □